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Modelling of deposition of flexible fractal-like aggregates on cylindrical fibre in continuum regime

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ABSTRACT

A new mathematical model of aggregate composed of *N* primary spherical particles has been created. The aggregate structure is modelled as an elastic body, capable of undergoing stretching, bending and twisting, during its movement in fluid. An aggregate is defined as a system of spherical particles joined together by springs, and the stiffness of structure is maintained by potential energy functions. Aggregate movement has been tracked in a Kuwabara cell model for three different values of velocity in continuum regime. The deposition efficiency of aggregates on a cylindrical collector has been related to the fractal dimension of aggregates, velocity of air and spring constant, which determine the magnitude of deformation of the aggregate structure. It was found that fractal dimension, velocity of air and imposed parameters of oscillations constants, strongly influence the deposition efficiency of aggregates.

1. Introduction

Aerosol aggregates are composed of many solid particles, and are of great concern in most environmental issues nowadays (Wichmann & Peters, 2000). Those aggregates which are created in diesel engines mostly affect the lungs, causing devastating irreversible consequences to human health as a result. International Agency of Research Cancer (IARC) has classified those aggregates as carcinogenic for humans. On their surface, aggregates can contain hazardous chemicals (Bünger et al., 2000), which are delivered deep into the respiratory system. One of the techniques, which deal effectively with the aggregates separation process from air, is filtration. The production of effective working filters needs to be enhanced by mathematical modelling of the filtration process. One of the crucial stages of computational simulations is to build up a fine mathematical model of the aggregate, which would include the interaction between primary particles.

Real aggregates may undergo modifications of structure owing to the fluid–structure interaction during their movement in fluid. This fact has explicit importance in estimating aggregates deposition ratios on the fibre of the filters. In order to establish deposition efficiencies for fractal-like aggregates, one should include interactions between primary particles which are often not stiff. Aggregates' deposition efficiency is determined largely by the deformation of their structure. A flexible or rigid structure of aggregate gives different values of deposition efficiency (Podgórski et al., 1995). The aim is to develop a model of an aggregate, which should consider interactions between primary particles and deformation of structure.

With the increasing power of the computers, research into the dynamics of fractal-like aggregates has been enhanced by more complex and accurate mathematical models of aggregates. There are two ways to model fractal-like aggregates.

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Nomenclature

$\boldsymbol{A}$	normal vector of plane created by triplet of particles *i–j–k*
$\boldsymbol{B}$	normal vector of plane created by triplet of particles *j–k–l*
d_p	diameter of primary particle in aggregate [m]
d_f	diameter of fibre [m]
C_S	Cunningham's slip correction factor
D	diffusion coefficient [m^2/s]
D_f	fractal dimension
$\widehat{\boldsymbol{e}}_x$, $\widehat{\boldsymbol{e}}_y$, $\widehat{\boldsymbol{e}}_z$	unit base vectors
E_I	efficiency of deposition of impaction mechanism
E_R	efficiency of deposition of interception mechanism
E_d	efficiency of deposition of diffusion mechanism
E	total efficiency of deposition considering all mechanisms
f_i	correction factor for drag force
f_d	damping factor of oscillations [kg/s]
f_d^*	dimensionless damping factor of oscillations
$f_{sh\ i}$	accessibility factor
$\boldsymbol{F}$	vector between connected particles *i* and *j*
$\boldsymbol{F}_i^B$	Brownian force acting on *i*th particle [N]
$\boldsymbol{F}_i^{D^*}$	drag force acting on *i*th particle [N]
$\boldsymbol{F}_i^s$	oscillation force acting on *i*th particle [N]
$\boldsymbol{F}_i^b$	bend force acting on *i*th particle [N]
$\boldsymbol{F}_i^t$	torsion force acting on *i*th particle [N]
$\boldsymbol{F}_i^p$	inverse force acting on *i*th particle [N]
$\boldsymbol{F}_i^{B*}$	Brownian force acting on *i*th particle [N]
$\boldsymbol{F}_i^{s*}$	dimensionless harmonic oscillation force acting on *i*th particle
$\boldsymbol{F}_i^{b*}$	dimensionless harmonic bend force acting on *i*th particle
$\boldsymbol{F}_i^{t*}$	dimensionless harmonic torsion force acting on *i*th particle
$\boldsymbol{F}_i^{p*}$	dimensionless harmonic inverse force acting on *i*th particle
$\boldsymbol{G}$	vector between connected particles *j* and *k*
$\boldsymbol{H}$	vector between connected particles *h* and *k*
J	parameter in the correlation function for efficiency of deposition of impaction mechanism.
k	Boltzmann's constant [J/K]
k_s	bond constant (spring constant) [kg/s^2]
k_b	bending constant [kg m/s^2]
k_t	torsion constant [kg m/s^2]
k_p	inversion constant [kg m/s^2]
Kn	Knudsen number
Ku	Kuwabara hydrodynamic factor
$\tilde{l}$	characteristic length [m]
m	parameter in interception mechanism
m_{pi}	mass of *i*th particle in aggregate [kg]
$\tilde{m}$	characteristic mass [kg]
n_i	number of neighbour particles (coordination number) of *i*th particle in aggregate
N	number of particles in aggregate
N_R	interception parameter
Pe	Peclet number
r_i	position of *i*th particle relatively to the origin of coordinate system [m]
r_{ij}	distance between particles indexed *i* and *j* respectively [m]
r_{0ij}	distance between two particles *i* and *j* in equilibrium state [m]
R_g	radius of gyration [m]
R_p	radius of primary particle in aggregate [m]
R_{max}	maximal radius of aggregate [m]
R_f	fibre radius [m]
R_{agg}	radius of fractal aggregate used as a radius of spherical particle [m]
Stk	Stokes number
t	time [s]
$\tilde{t}$	characteristic time [s]
T	temperature of fluid [K]
$V_s(r_{ij})$	harmonic bond potential energy [J]
$V_b(\theta_{ijk})$	harmonic cosine angle potential energy [J]
$V_t(\varphi_{ijkl})$	torsion potential energy [J]
$V_p(\xi_{ijkl})$	inversion potential energy [J]
$\boldsymbol{v}_i$	velocity of *i* particle in aggregate [m/s]
$\boldsymbol{v}_i^*$	dimensionless velocity of *i*th particle in aggregate
U	velocity of ambient air around cylindrical collector [m/s]
U^*	dimensionless velocity of ambient air around cylindrical collector
$\boldsymbol{Z}_i$	dimensionless vector, with random direction and magnitude that is distributed normally, with zero mean and unit variance.

Greek letters

α	packing density of filter structure
α_{Be}	characteristic magnitude of the acceleration of Brownian excitation[m/s^2]
α_{vB}	characteristic magnitude of the deceleration caused by viscous dissipation during the Brownian motion of a single primary particle [m/s^2]
$\delta_{\alpha\beta}$	Kronecker delta symbol
$\epsilon_{\alpha\beta\gamma}$	Levi–Civita symbol
Δt	time step used to integrate equation of trajectory [s]
Δt^*	dimensionless time step used to integrate equation of trajectory
η	deposition efficiency of aggregates
θ_{ijk}	angle created between vectors of two pairs of particles *i–j* and *j–k*
θ_{0ijk}	initial angle created between vectors of two pairs of particles *i–j* and *j–k*
μ_f	viscosity of fluid [Pa s]
ξ_{ijkl}	angle between plane created by triplet of particles *i–j–k* and vector created by particles *j–l*
ξ_{0ijkl}	initial angle between plane created by triplet of particles *i–j–k*, and vector created particles *j–l*
ρ	density of fluid [kg/m^3]
ρ_p	density of aggregate particle [kg/m^3]